

# Soil & Water Chemistry Research

## **Soil & Water Chemistry Research**

**D. L. Suarez**  
**Research Leader**

### **Secretary**

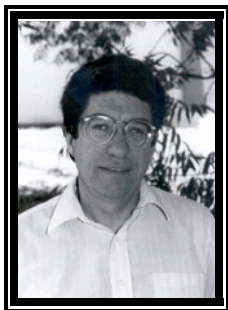
**JoAnne Rose Coons**

**D. Corwin - Soil Scientist**  
**H.S. Forster - Phys. Sci. Tech.**  
**S. Goldberg - Soil Scientist**  
**R. LeMert - Sr. Farm Machinery Mechanic**  
**S. Lesch - Sr. Statistician**  
**I. Lebron - Soil Scientist**  
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**N. Vishteh - Biol. Sci. Tech.**  
**J.D. Wood - Soil Scientist**

## **Mission**

The mission of the Soil & Water Chemistry unit is to elucidate and quantify the chemical processes operative in salt-affected and/or sodic soils, including toxic elements; to develop instrumentation and technology for salinity measurement; and to develop control practices and agricultural management technologies to sustain irrigation while conserving soil and water resources. Major emphasis is to (1) develop models of the chemical and mineralogical controls of soil rootzones water compositions and (2) develop instrument-, tracer-, and GIS-techniques for the assessment and management of soil salinity and the determination of sources and magnitudes of salt loading. The specific objectives of the research program are to: (1) develop models and comprehensive criteria/standards to assess the suitability of salt-affected water for irrigation; (2) develop reclamation models; (3) develop knowledge necessary to predict mobility of potentially toxic trace anions, such as B, As, Se and Mo, in irrigated rootzones; (4) develop a methodology which uses geophysical measurements and image processing techniques to estimate the source and magnitude of salt discharges from irrigated soil; and (5) develop a GIS, and functional transport models to predict field-scale distributions of solute loading to groundwater.

## SOIL & WATER CHEMISTRY RESEARCH STAFF



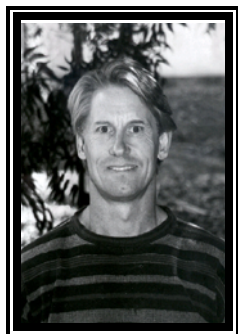
**DONALD L. SUAREZ, B.A., Ph.D., Research Leader and Supervisory Geologist of the Soil & Water Chemistry Research.**

Water quality criteria for irrigation, predicting groundwater quality in relation to agricultural practices, modeling solute transport in soils, structural stability and reclamation of sodic soils and impact of irrigation on inorganic carbon budgets.



**SABINE GOLDBERG, B.S.A., Ph.D. Soil Scientist for Soil & Water Chemistry Research.**

Trace elements adsorption reactions for predicting interactions with soil water in the irrigated root zone, chemical effects of salts on soil physical properties, structural stability of sodic soils.



**DENNIS L. CORWIN, B.S., Ph.D., Soil Scientist for Soil & Water Chemistry Research.**

Development of management-oriented solute transport models to determine solute loading to the groundwater; measurement and assessment of soil salinity for the purpose of irrigation and drainage management; integration of solute transport models and geographic information systems for regional scale assessments and predictions of solute loading to the groundwater.

**JAMES D. RHOADES, B.S., M.S., Ph.D., Supervisory Soil Scientist for Soil & Water Chemistry Research.**

Use of saline waters for irrigation; assessment of adequacy of leaching and drainage for salinity control; assessment of suitability of water for irrigation; soil salinity appraisal using geophysical instrumentation and use to assess the appropriateness of irrigation/drainage practices; and management to control pollution from irrigation/drainage.



**CHUNMING SU, B.S.C., M.S., Ph.D., Soil Scientist for Soil & Water Chemistry Research.**

Partitioning of trace elements at interfaces between soil minerals and water; weathering of minerals in saline soils, and determination of B, Se and Mo speciation on oxide surfaces using FTIR.

## **EVALUATION OF A SIMPLE LYSIMETER-DESIGN MODIFICATION TO MINIMIZE SIDEWALL FLOW**

**D.L. Corwin**

A common criticism of many soil lysimeter designs has been the existence of artificial flowpaths along the soil-wall interface. This artificial flow is referred to as sidewall flow. A simple lysimeter-design modification was evaluated that utilizes annular rings to divert sidewall flow near the soil surface into the soil column to minimize the occurrence of sidewall flow along the remainder of the column's length. A chloride-tracer experiment was used to evaluate the effectiveness of annular rings in minimizing sidewall flow in a mesoscale soil lysimeter (0.6 m in diameter and 1.83 m in height). The tracer-experiment data showed that even though sidewall flow may not have been completely eliminated it was reduced to an undetectable level based on chloride distributions and time domain reflectometry measurements. However, a delicate balance exists between minimizing sidewall flow and significantly altering the natural water-flow dynamics when using annular rings. The simple design modification provides a means of using a disturbed column of soil to evaluate models of solute transport, and to study preferential flow and contaminant mobility without concern for spurious data due to artificial flow along the soil-wall interface of the lysimeter.

Journal of Contaminant Hydrology, 42:35-49, 1999.

## **EVALUATION OF A GIS-LINKED MODEL OF SALT LOADING TO GROUNDWATER**

**D.L. Corwin, M.L.K. Carrillo, P.J. Vaughan, D.G. Cone and J.D. Rhoades**

The ability to assess through prognostication the impact of nonpoint source (NPS) pollutant loads to groundwater, such as salt loading, is a key element in agriculture's sustainability by mitigating deleterious environmental impacts before they occur. The modeling of NPS pollutants in the vadose zone is well suited to the integration of a geographic information system (GIS) because of the spatial nature of NPS pollutants. The GIS-linked, functional model TETrans was evaluated for its ability to predict salt loading to groundwater in a 2396 ha study area of the Broadview Water District located on the westside of central California's San Joaquin Valley. Model input data were obtained from spatially-referenced measurements as opposed to previous NPS pollution modeling effort's reliance upon generalized information from existing spatial databases (e.g., soil surveys) and transfer functions. The simulated temporal and spatial changes in the loading of salts to drainage waters for the study period 1991-1996 were compared to measured data. A comparison of the predicted and measured cumulative salt loads in drainage waters for individual drainage sumps showed acceptable agreement for management applications. An evaluation of the results indicated the practicality and utility of applying a one-dimensional, GIS-linked model of solute transport in the vadose zone to predict and visually display salt loading over thousands of hectares. The display maps provide a visual tool for assessing the potential impact of salinity upon groundwater, thereby providing information to make management decisions for the purpose of minimizing environmental impacts without compromising future agricultural productivity.

J. Environ. Qual. 42(2):471-480, 1999.

## **EVALUATION OF A FUNCTIONAL MODEL FOR SIMULATING BORON TRANSPORT IN SOIL**

**D.L. Corwin, S. Goldberg and A. David**

There has been renewed interest in the application of functional models to the transport of nonpoint source pollutants at polypedon (i.e., farm) and watershed scales due to the ease of their coupling to a geographic information system and to the accepted organizational hierarchy of pedogenetic modeling approaches. However, very little work has been done to closely evaluate the performance of a functional transient-state model for the transport of a reactive solute over an extensive study period. The functional model TETrans was evaluated for model performance with boron (B) transport data collected from a soil lysimeter column over a 1000-day study period. Because the ability to simulate water flow has been previously evaluated for TETrans, the focus of this evaluation centered around the performance of various functional models of B adsorption used as subroutines within the TETrans model including the (1) Freundlich, (2) kinetic Freundlich, (3) Langmuir, (4) temperature-dependent Langmuir, and (5) pH-dependent Keren adsorption isotherm equations. Model performance was evaluated with statistical functions, and graphic displays of observed and predicted B concentration profiles. Results indicated that the order of model performance was the pH-dependent Keren equation first, followed by the kinetic Freundlich and Freundlich equations, the temperature-dependent Langmuir equation, and finally the Langmuir equation. Overall, the TETrans model was able to simulate the transport of B with deviations attributed to the fact that no functional adsorption equation incorporated all the influences of pH, ionic strength, temperature and kinetic effects into a single equation.

Soil Science 164(10):697-717, 1999.

## **ADVANCED INFORMATION TECHNOLOGIES FOR ASSESSING NONPOINT SOURCE POLLUTION IN THE VADOSE ZONE: CONFERENCE OVERVIEW**

**D.L. Corwin, K. Loague and T.R. Ellsworth**

The information age has ushered in an awareness of and concern for global environmental problems such as climatic change, ozone depletion, deforestation, desertification, and nonpoint source (NPS) pollution. Nonpoint source pollution is the single greatest threat to surface and subsurface drinking water resources. Nonpoint source pollutants also pose a threat to sustainable agriculture, which is viewed as the most viable means of meeting the food demands of a world population that is expected to reach 9.4 billion by the middle of the next century. The ability to accurately assess present and future NPS pollution impacts on ecosystems ranging from local to global scales would provide a powerful tool for environmental stewardship and guiding future human activities. Assessing NPS pollutant is a multidisciplinary problem. To address the problem, advance information technologies and methodologies are needed that draw from all areas of science and are applied in a spatial context. It was from this setting that the 1997 Joint AGU Chapman/SSSA Outreach Conference *Application of GIS, Remote Sensing, Geostatistics, and Solute Transport Modeling for Assessing Nonpoint Source Pollutants in the Vadose Zone* (19-24 October 1997, Riverside, CA) materialized. The objective of the conference was to examine current multidisciplinary technologies and methodologies for assessing NPS pollutants in the vadose zone, and to explore new conceptual approaches. It was the conference's goal to provide a forum to stimulate multidisciplinary interactions to enhance the development of techniques for the realtime measurement and modeling of NPS pollution in the vadose zone and subsurface waters.

J. Environ. Qual. 28(2):357-365, 1999.

## **REGIONAL SCALE ASSESSMENT OF NON-POINT SOURCE GROUNDWATER CONTAMINATION**

**K. Loague and D.L. Corwin**

Predictive assessments of non-point source (NPS) pollution can have great utility for environmentally focused land use decisions related to both the remediation of existing groundwater contamination and the regulation of current (and future) agrochemical use. At the regional scales associated with NPS agrochemical applications there are staggering data management problems in assessing potential groundwater vulnerability. Geographical information system (GIS) technology is a timely tool that greatly facilitates the organized characterization of regional-scale variability. In this paper we review the recently reported (Loague et al., 1988a,b) simulations of NPS groundwater vulnerability, resulting from historical applications of the agrochemical DBCP (1,2-dibromo-3-chloropropane), for east-central Fresno County (California). The Fresno case study helps to illustrate the data requirements associated with process-based three dimensional simulations of coupled fluid flow and solute transport in the unsaturated/saturated subsurface at a regional scale. The strengths and weaknesses of using GIS in regional-scale vulnerability assessments, such as the Fresno case study, and the critical problem of estimating the uncertainties in these assessments (owing to both data and model errors) are discussed. A regional GIS-driven integrated assessment approach is proposed, which is based upon cost-benefit analysis, and incorporates both physical and economic factors that can be used in a regulatory decision process.

In: A.M. Gurnell and D.R. Montgomery (eds). *“Hydrological Applications of GIS”*, John Wiley & Sons, Chapter 10 p.137-145, 2000.



## **INVERSION OF SOIL CONDUCTIVITY PROFILES FROM ELECTROMAGNETIC INDUCTION MEASUREMENTS: 2. EXPERIMENTAL VERIFICATION**

**J.M.H. Hendrickx, J.D. Rhoades, D.L. Corwin, S.M. Lesch, A.C. Hilgendorf  
and B. Borchers**

Non-invasive electromagnetic (EM) induction techniques are increasingly being used for salinity monitoring of agricultural lands and contaminant detection in soils and shallow aquifers. The physical relationships between the apparent electrical conductivity ( $EC_a$ ) of a homogeneous semi-infinite half space and the response of an EM ground conductivity meter are well understood. Although theoretical considerations indicate the validity of these depth response functions or forward models for heterogeneous profiles, no experimental data have been presented to verify this assumption. The objectives of this study are twofold. The first one is to experimentally verify whether the linear and non-linear electromagnetic forward models for homogeneous media are valid in heterogeneous soil profiles. The second objective is the experimental verification of linear and non-linear methods for inversion of soil conductivity profiles using above-ground electromagnetic induction measurements with the EM38 ground conductivity meter. Experimental data from fourteen representative saline soil profiles in California have been used for the verification of linear and non-linear forward and inverse models. The linear and non-linear forward models derived for homogeneous media are indeed valid in heterogeneous soil profiles. However, since the errors of the linear forward model are approximately double those of the non-linear forward model, the latter is the preferred one. No such difference was found between the linear and non-linear inverse models. In this study the linear inverse model outperforms the non-linear model at EM38 measurements below 150 mS/m while at higher conductivities the non-linear inverse model yields slightly better results. The linear model is preferred since it needs considerably less computer resources.

## **SOLUTE CONTENT - SUCTION CUPS, POROUS MATRIX SENSORS, ELECTRICAL RESISTIVITY**

**J. M. Hendrickx, D.L. Corwin, J. Wraith and R.G. Kachanoski**

Soil consists of solid, liquid, and gas phases. The measurement of the solute content of the soil solution is a quantification of the chemicals that are present in the liquid portion of the soil. This provides a means of determining the level of contamination and degradation status of the soil. The liquid phase of the soil is significant because it allows contaminants to move through the soil via diffusion or mass transport. A discussion of the principles, equipment, procedure and comments regarding the measurement of solutes in the soil solution with suction cups, porous matrix sensors and electrical resistivity is presented. The discussion is part of the Solute Content Chapter of the Soil Science Society of America's Agronomy Monograph No. 9 Methods of Soil Analysis 3rd Edition. The discussion is designed to provide researchers with the background, latest equipment, and current accepted procedures and methodology for measuring solute concentration in the soil solution (particularly of soil salinity) with suction cup extractors, porous matrix/salinity sensors, and electrical resistivity.

SSSA Agronomy Monograph #9, Methods of Soil Analysis (3rd Edition) Chapter 6.1. 2000.

## **SIMULATING MOLYBDENUM TRANSPORT THROUGH THE ROOT ZONE IN A SOIL LYSIMETER**

**D.L. Corwin, S. Goldberg and A. David**

Due to the ease of their coupling to a geographic information system and to the accepted organizational hierarchy of pedogenic modeling approaches, there has been renewed interest in the application of functional models to the transport of non-point source pollutants. A functional model of solute transport was used to simulate molybdenum movement through a mesoscale soil lysimeter column (0.6 m diameter, 1.83 m length) over a 1000-day study period. The focus was upon a comparison of the performance of various functional models of molybdenum adsorption used within the transport model including the (1) Freundlich, (2) kinetic Freundlich, (3) Langmuir, (4) temperature-dependent Langmuir, and (5) ph-dependent adsorption isotherm equations. Measured and simulated distributions of soil solution molybdenum were compared at depths of 0.15, 0.45, 0.75, 1.05 and 1.35 m. The model was best able to simulate the transport of molybdenum at the intermediate depths of 0.45 and 0.75 m and to a lesser extent the deeper depths of 1.05 and 1.35m, but was unable to reliably predict the shallowest depth. Failure to predict the shallowest depth was attributed to the methodology, specifically the inability to consistently collect soil solution extracts at field capacity.

Agronomy Abstract p. 345, 1999.

## **DETECTION OF SOIL SALINITY EFFECTS ON SUGAR BEETS USING MULTISPECTRAL REMOTE SENSING**

**G.J. Fitzgerald, S.R. Kaffka, D.L. Corwin, S.M. Lesch and S.J. Maas**

High resolution multi spectral remotely sensed imagery was acquired on four dates during the 1999 growing season for sugar beet field near Stratford, California using the Shafter Airborne Multispectral Remote Sensing System (SAMRSS), a digital airborne imaging system developed by the USDA-ARS laboratory at Shafter, CA. It consists of three digital cameras fit with specially coated filters allowing narrow band transmission of light at 550nm (green), 660 nm (red), and near infrared (850nm) wavelengths. Ground soil salinity was measured based on soil electrical resistivity measurements taken at over 3100 locations in the 160 acre study area. A soil salinity map of the field was generated using the resistivity measurements and associated soil core samples taken at 1 foot increments down to 4 feet at 19 statistically selected locations. Yield data were collected in small plots for root quality determinations and with a yield monitor mounted on a sugar beet harvester to estimate root yield. These data were correlated to the images collected to determine relationships between the images, soil salinity, and yield.

Agronomy Abstract p. 17, 1999.

## **SOIL EC THEORY AND PRINCIPLES: WHAT IS IT AND HOW DOES IT WORK?**

**D.L. Corwin**

A general overview of the measurement of soil salinity using various electrical conductivity (EC) measurement techniques (i.e., soil-matrix salt sensors; electrical resistivity methods such as four-electrode probe and Wenner array; and electromagnetic induction) is presented with particular emphasis on spatial EC measurements. The following areas are discussed in the overview: brief history of the measurement of soil salinity, basic theories and principles of soil electrical conductivity measurement, electrical conductivity measurement techniques, examples of spatial EC measurement studies, applications and value of spatial measurements of soil EC to precision agriculture, and current/future developments.

Agronomy Abstract p. 77, 2000.

## **FIELD SCALE ELECTRICAL CONDUCTIVITY AND CROP PRODUCTION IN CALIFORNIA**

**S.R. Kaffka, D.L. Corwin and S.M. Lesch**

There has been little assessment of yield variation at the field scale in California. Two salt-affected fields, one in the Imperial Valley (IV) and one in the San Joaquin Valley (SJV), were assessed under uniform moisture conditions using electromagnetic induction (EM) methods and planted to sugarbeets. Both field scale yield maps and hand samples from sites identified based on survey data using a multiple regression algorithm were derived. Electrical conductivity (ECe) varied from 2 to 9 dS m<sup>-1</sup> at the IV site, and from 3 to 24 dS m<sup>-1</sup> at the SJV site. Percent seedling establishment declined from approximately 70% to 40% over the ECe range observed. Sugar yields varied within the field from 13.4 to 17.7 Mg ha<sup>-1</sup>, but was not significantly correlated with ECe. Sucrose concentration in roots increased significantly from 16.4 to 19.3 mg kg<sup>-1</sup> in response to increasing ECe. At the SJV site, root and sucrose yield (2.9 to 14.2 Mg ha<sup>-1</sup>) responded more to soil texture, represented by soil saturation percentage (SP), but was positively correlated with ECe. Sucrose concentration varied from 15.0 to 18.7 mg kg<sup>-1</sup>, but was not affected by ECe. Different sugarbeet responses to ECe at the two sites are related to irrigation methods and more difficult management conditions at the SJV site.

Agronomy Abstract p. 80, 2000.

## **THE INFLUENCE OF SALINITY ON SPATIAL VARIABILITY OF 13C NATURAL ABUNDANCE IN PLANT AND SOIL**

**J.W. Van Groenigen, D.L. Corwin, W.R. Horwath and C. Van Kessel**

Salinity-induced stress will cause plants to partially close their stomata. This will lead to a relative enrichment with  $^{13}\text{C}$ , and corresponding higher  $[\delta]^{13}\text{C}$  values in organic matter. The objective of this study was to explore the possibility of using differences in  $[\delta]^{13}\text{C}$  values in plant and soil organic (SOM) fractions to reconstruct the salinity history of a field. We compared spatial patterns of salinity,  $[\delta]^{13}\text{C}$  of the SOM and  $[\delta]^{13}\text{C}$  of crops on a Lethent Clay Loam in San Joaquin Valley, California. The ECa values ranged from 3 to 18 dS m<sup>-1</sup> and  $[\delta]^{13}\text{C}$  values of the crop and SOM ranged from -29.8 to -24.0‰ and -25.3 to -21.4‰, respectively. Spatial patterns of salinity and  $[\delta]^{13}\text{C}$  crop was highly correlated, with higher  $[\delta]$  values associated with higher salinity. There was no relation between salinity and  $[\delta]^{13}\text{C}$  SOM patterns. Therefore we concluded that current salinity is likely of recent origin. To verify this conclusion, the  $[\delta]^{13}\text{C}$  pattern of the light SOM fraction, which is considered to be the youngest SOM pool, should reflect the spatial salinity pattern. By distinguishing between  $[\delta]^{13}\text{C}$  values of the light

SOM fraction and older physical or chemical SOM fractions, the historic pattern of salinity stress can be reconstructed.

Agronomy Abstract p. 309, 2000.

## **FIELD-SCALE SOIL ELECTRICAL CONDUCTIVITY CHARACTERISTICS AND SUGARBEET EMERGENCE, GROWTH, AND YIELD**

**S. R. Kaffka, D. L. Corwin, S. M. Lesch and G. Fitzgerald**

An assessment of field-scale variation and the characterization of correlated crop response to this variation are first steps in evaluating the potential for variable rate technologies and other aspects of precision agriculture. As an initial attempt at site characterization, the response of sugarbeets to salinity and residual nitrogen was studied at sites in the Imperial and San Joaquin Valleys. Evaluation of the usefulness of salinity assessment technology developed by Rhoades and fellow workers at the U.S. Salinity Laboratory for precision agricultural management and the possible correlation of salinity and nitrate, especially deeper in the soil profile, were the objectives of this study. Nitrate was found to correlate with  $EC_e$  and  $EC_a$  (electrical conductivity of the saturation paste and bulk soil, respectively) at depth. This means that higher  $EC_a$  values can be used as a means of identifying likely locations in the profile to sample for residual  $NO_3-N$ . For sugarbeets, nitrate deep in the soil profile can lead to reduced sugar concentrations in the roots. The use of soil electrical conductance to evaluate variation in soil residual nitrate may make field scale assessment for this purpose far less expensive and much more practical and accurate than other ground-based attempts reported previously, and allow for sufficient amounts of data to be collected to make precision agricultural practices profitable.

Proceedings California Plant & Soil Conference, Stockton, CA, Abstr. p. 17, 2000.



# **REANALYSIS OF BORON ADSORPTION ON SOILS AND SOIL MINERALS USING THE CONSTANT CAPACITANCE MODEL**

**S. Goldberg**

The constant capacitance model is shown to provide a quantitative description of boron adsorption on various aluminum and iron oxides, clay minerals, and arid zone soils as a function of solution pH. In the present model application, both trigonal and tetrahedral boron surface complexes are postulated, consistent with experimental spectroscopic results. Average sets of boron surface complexation constants for aluminum and iron oxides and kaolinites are not statistically significantly different from each other. Average sets of boron surface complexation constants for kaolinites are statistically significantly different from those for 2:1 clays and soils. Average sets of boron surface complexation constants for 2:1 clays and soils are not statistically significantly different from each other reflecting the dominance of 2:1 clay minerals in boron adsorption reactions in these arid zone soils. Average sets of boron surface complexation constants provided adequate descriptions of boron adsorption behavior on all adsorbents studied, indicating some predictive capability. The constant capacitance model was able to predict boron adsorption behavior on additional arid zone soils using the average set of boron surface complexation constants.

Soil Sci. Soc. Am. J. 63(4):823-829, 1999.

## **SOIL COLLOIDAL BEHAVIOR**

**S. Goldberg, I. Lebron and D.L. Suarez**

Recent understanding that organic and inorganic contaminants are often transported via colloidal particles has increased interest in colloid science. The primary importance of colloids in soil science stems from their surface reactivity and charge characteristics. Characterizations of size, shape, surface area, and surface charge density are required for understanding the processes of adsorption, flocculation, dispersion, and transport in soils and the resultant changes in soil hydraulic properties as well as chemical migration. Colloids are reactive not only because of their total surface area but because of enhanced reactivity related to rough surfaces and highly energetic sites, as well as the effects of electrostatic charge. Colloid charge is associated with substitution of lower charge cations for those of higher charge in the mineral lattice as well as surface charge associated with broken bonds. The charge associated with broken bonds is characterized as variable charge in as much as the solution influences the surface speciation. In addition to these chemical processes, colloids are mobile in soils and thus affect not only the chemical transport of otherwise immobile chemicals but also exert a strong influence on soil hydraulic properties. Prediction of transport of pathogens (viruses and bacteria), radionuclides, heavy metals and organic contaminants require consideration of colloid mobility and thus understanding of both physical processes as well as surface chemistry. We review the general principles pertaining to these processes.

In: Malcolm E. Sumner (ed.) *"Handbook of Soil Science"*, Section II, Soil Chemistry, Chapter 6, p. B195-B240, CRC Press, Boca Raton, FL, 1999.

## **PREDICTING BORON ADSORPTION BY SOILS USING SOIL CHEMICAL PARAMETERS IN THE CONSTANT CAPACITANCE MODEL**

**S. Goldberg, S.M. Lesch and D.L. Suarez**

The constant capacitance model, a chemical surface complexation model, was applied to B adsorption on 17 soils selected for variation in soil properties. A general regression model was developed for predicting soil B surface complexation constants from easily measured soil chemical characteristics. These chemical properties were cation-exchange capacity (CEC), surface area, organic carbon content (OC), and inorganic carbon content (IOC). The prediction equations were used to obtain values for B surface complexation constants for 15 additional soils, thereby providing a completely independent evaluation of the ability of the constant capacitance model to fit B adsorption. The model was well able to predict B adsorption on the 15 soils. Incorporation of these prediction equations into chemical speciation-transport models will allow simulation of soil solution B concentrations under diverse environmental and agricultural conditions without the requirement of soil specific adsorption data and subsequent parameter optimization.

Soil Sci. Soc. Am. J. 64:1356-1363, 2000.

## **PREDICTION OF BORON ADSORPTION IN SOILS USING THE CONSTANT CAPACITANCE MODEL**

**S. Goldberg, S.M. Lesch and D.L. Suarez**

The constant capacitance model, a chemical surface complexation model, was applied to boron adsorption on 14 assorted arid-zone soil samples. In agreement with previous spectroscopic results, we specified both trigonal and tetrahedral surface configurations for adsorbed boron. A general regression model was developed for predicting soil boron surface complexation constants from easily measured chemical soil characteristics. These chemical properties were cation exchange capacity, surface area, organic carbon content, and inorganic carbon content. The prediction equations were used to obtain values of boron surface complexation constants for four independent soils. Since the data from the four soils had not been used to develop the prediction equations, this is a completely independent evaluation of the ability of the general regression model to predict boron adsorption. The model was well able to predict boron adsorption on additional arid-zone soils from the Central Valley of California. The data base has been expanded and the regression model will be refined by including 16 additional soils having broader ranges of chemical characteristics.

ENVR 118, 217th ACS National Meeting, Anaheim, CA, Abstr., 1999.

## **COMPETITIVE ADSORPTION OF ARSENATE AND ARSENITE SPECIES ON OXIDES AND CLAY MINERALS**

**S. Goldberg**

Arsenic is a toxic trace element for animals including humans. EPA proposes to significantly lower the As drinking water standard within the next year. Adsorption reactions on soil mineral surfaces potentially attenuate toxic soil solution As concentrations reducing contamination of groundwaters. Arsenic adsorption on amorphous aluminum and iron oxides and the clay minerals, kaolinite, montmorillonite, and illite was investigated as a function of solution pH and arsenic redox state. Arsenic adsorption experiments were carried out in batch systems to determine adsorption envelopes, amount of As(III) and/or As(V) adsorbed as a function of solution pH per fixed total As concentration. The constant capacitance model was able to fit the arsenate and arsenite adsorption envelopes to obtain values of the intrinsic As surface complexation constants. These intrinsic surface complexation constants were then used in the constant capacitance model to predict competitive arsenate-arsenite adsorption from solutions containing equimolar As(III) and As(V). The constant capacitance model was well able to predict As adsorption from mixed As(III)/As(V) solutions.

Agronomy Abstract p. 223, 2000.

# **SATURATED HYDRAULIC CONDUCTIVITY AS AFFECTED BY PORE SIZE AND PORE GEOMETRY IN SOILS WITH VARIABLE CHEMICAL COMPOSITION**

**I. Lebron, M.G. Schaap and D.L. Suarez**

The methodology presented in this work consists in the analysis of binary images collected with a back scattered electron detector from thin sections of soils. Maximum and average diameter, surface area, perimeter, roughness and circularity were quantified. Saturated hydraulic conductivity ( $K_{sat}$ ) was measured in 36 undisturbed soils, particle size distribution, particle density, bulk density and chemical properties were determined in half of the core, the other half was used to prepare thin sections. We used the Kozeny-Carman equation to predict  $K_{sat}$  from the microscopic measurements, and neural network analysis to predict the formation factor from microscopic, macroscopic, and chemical data. Formation factor was best predicted when % clay, bulk density, roughness, and pH were used in the neural network and bootstrap approach. The predicted  $K_{sat}$  was in excellent agreement with the measured  $K_{sa}$  ( $R^2=0.97$ ) when a hydraulic radius defined as  $r_H=area/perimeter$  was used. Area and perimeter are direct measurements obtained from the back scattered images. The improvement in our  $K_{sat}$  predictions when  $r_H$  is used instead of an average radius indicates that

the methodology proposed in this study may be useful to improve our capability to predict hydraulic properties.

Water Resources Research 35(10):3149-3158, 1999.

## MODELING CALCITE PRECIPITATION AS AFFECTED BY $P_{\text{CO}_2}$ AND ORGANIC LIGANDS AT 25°C

I. Lebron and D.L. Suarez

We found that the DOC affects both crystal growth and heterogeneous nucleation at the three  $P_{\text{CO}_2}$  values studied. The precipitation rate of calcite in the range of  $\omega = 2.5$ -20 decreased when the DOC concentration increased for  $P_{\text{CO}_2}$  0.035, 5, and 10 kPa, however higher DOC concentrations were needed to cause an equal reduction in the precipitation when the  $P_{\text{CO}_2}$  increased. Calcite precipitation studies are generally performed in clean systems and measure the effects of pH and  $P_{\text{CO}_2}$  on calcite precipitation at different temperatures for crystal growth. However, water soluble organic ligands and ions such as  $\text{PO}_4^{3-}$  have been known to act as precipitation inhibitors by blocking crystal growth sites. In a seeded crystal growth experiment Inskeep and Bloom (1986) found that the precipitation rate constant decreased to zero at  $\omega = 8$ -9 in the presence of 0.15 mM dissolved organic carbon (DOC) from a water-soil extract. Levels of DOC in natural environments are comparable to the levels found by Inskeep and Bloom (1986) to inhibit calcite precipitation. Lebron and Suarez (1996) incorporated the effect of the DOC in an equation to describe calcite precipitation. This model also includes a term for calcite precipitation by crystal growth and a term for calcite precipitation by heterogeneous nucleation. This is the only model in the literature that attempted to reproduce calcite precipitation in natural environments however, this model was developed only for atmospheric partial pressure of  $\text{CO}_2$ . It is well known that concentrations of  $\text{CO}_2$  in the root zone are 10-500 times higher than in the atmosphere. With that in mind, the objectives of the present study are: (1) To determine the effect of DOC on crystal growth and heterogeneous nucleation of calcite at different levels of  $P_{\text{CO}_2}$ ; and (2) To quantify the effect of  $P_{\text{CO}_2}$  and DOC concentration in a precipitation rate model.

Mineralogical Magazine 62A:864-865, 1999.

## **MECHANISMS AND PRECIPITATION RATE OF RHODOCHROSITE AT 25°C AS AFFECTED BY $P_{\text{CO}_2}$ AND ORGANIC LIGANDS**

**I. Lebron and D.L. Suarez**

Rhodochrosite is the main Mn mineral phase in neutral to alkaline anoxic environments and is likely the initial precipitation phase when  $\text{Mn}^{2+}$  is added to irrigation water. Solutions supersaturated with respect to rhodochrosite that was detected in various natural environments suggest that equilibrium assumptions may not be satisfactory and kinetic processes may be dominant. This study was conducted to evaluate the precipitation mechanisms of rhodochrosite in natural environments where DOC is present and there are variations in partial pressure of  $\text{CO}_2$  ( $P_{\text{CO}_2}$ ). Precipitation rates were measured in supersaturated solutions of rhodochrosite in the presence of seeds of the mineral and  $P_{\text{CO}_2}$  0.035 kPa, 5 kPa, and 10 kPa and in a concentration range of DOC of 0.02 to 3.2 mM of Suwannee River fulvic acid. Precipitation rates were measured in the absence and presence of 1 mM leonardite humic acid. Precipitation rates increased when the  $P_{\text{CO}_2}$  increased and decreased when the concentration of the fulvic acid increased at constant levels of supersaturation. However, higher concentrations of DOC were needed to produce the same reduction in precipitation rates when  $P_{\text{CO}_2}$  was increased. The most likely causes of the increase in the precipitation rate when  $P_{\text{CO}_2}$  increases are an increase in the negative surface charge and an increase in the activity of  $\text{MnHCO}_3^+$ . No significant change in the precipitation rate of rhodochrosite was measured when the leonardite humic acid was added to the reaction vessels. The lack of inhibition of leonardite humic acid on rhodochrosite precipitation is explained by its molecular configuration in solution.

Soil Sci. Soc. Am. J. 63(3):561-568, 1999.



# **SATURATED HYDRAULIC CONDUCTIVITY PREDICTION FROM MICROSCOPIC PORE GEOMETRY MEASUREMENTS AND NEURAL NETWORK ANALYSIS**

**I. Lebron, M.G. Schaap and D.L. Suarez**

Flow and transport of water and solutes in soils are controlled by the size, geometry and characteristics of the soil porosity. Most of the characteristics of soil pores are microscopic, such as roughness and circularity. Conventional models of liquid distribution, flow and solute transport rely solely on cylindrical capillarity ignoring the role of surface area, angularity, and connectivity. This study was conducted to develop a new methodology to directly measure the porosity and its microscopic characteristics. The methodology is based on the analysis of binary images collected with a backscattered electron detector from thin sections of soils. Pore surface area, perimeter, roughness, circularity, and maximum and average diameter were quantified in 36 thin sections prepared from undisturbed soils. Saturated hydraulic conductivity ( $K_{sat}$ ), particle size distribution, particle density, bulk density and chemical properties were determined on the same cores. We used the Kozeny-Carman equation, neural network and bootstrap analysis to predict a formation factor from microscopic, macroscopic, and chemical data. The predicted  $K_{sat}$  was in excellent agreement with the measured  $K_{sat}$  ( $R^2=0.91$ ) when a hydraulic radius defined as  $r_H$ =pore area/pore perimeter and the formation factor were included in the Kozeny-Carman equation.

AGU Conference, vol. 80(46)F370, San Francisco, CA, Abstr., 1999.

## **SOIL PORE SPACE AS AFFECTED BY SODIUM**

**I. Lebron, D.L. Suarez and M.G. Schaap**

Soil porosity and texture are important properties affecting the soil hydraulic properties. Using scanning electron micrographs and image analysis we quantified the actual pore and aggregate size distribution in undisturbed soil cores. We observed, for soils with similar texture, a decrease in the average aggregate size and in the aggregate size distribution when the sodium content in the soil increased and when the pH increased. The cementing agents binding the domains conforming the aggregates were hypothesized to be responsible for the decrease in the aggregate stability. Equivalent decrease in the pore size distribution was found with increasing sodium and pH. There was a significant correlation between average aggregate size and average pore size, but not relationship between average pore diameter and texture. The use of aggregate size distribution instead of soil texture improved the saturated hydraulic conductivity predictions using a pedotransfer function based code.

Agronomy Abstract p. 212, 2000.

# **MOBILIZED SOIL CONDUCTIVITY ASSESSMENT SYSTEMS: AN OVERVIEW OF SOME COMMON SYSTEM DESIGN AND DATA INTERPRETATION ISSUES**

**S. M. Lesch**

Mobilized soil conductivity assessment (MSCA) systems have been used approximately ten years now for the purposes of mapping and monitoring field-scale spatial soil salinity patterns (Rhoades, 1992). More recently, MSCA systems have been increasingly used to map and/or categorize a wide range of physical/chemical soil properties. This increase in the use and acceptance of such systems is directly related to the current interest in acquiring rapid, accurate precision farming related information. This article presents a brief overview of some pertinent MSCA system design and data interpretation issues. Included here is a review of the basic MSCA system components, some simple system integration concepts, and a general summary of the most commonly used methods for interpreting, modeling, and/or calibrating soil conductivity survey data.

Proceedings 1999 California Plant and Soil Conference. Agricultural Technology - Moving California into the 21st Century. California Chapter of American Society of Agronomy and California Fertilizer Association, 1999.

# **THE ESAP-95 VERSION 2.01R USER MANUAL AND TUTORIAL GUIDE**

**S.M. Lesch, J.D. Rhoades and D.L. Corwin**

This manual describes and documents a series of site selection and salinity modeling software programs, collectively known as the ESAP-95 software package (Release version 2.01R), developed for the analysis and prediction of soil salinity from conductivity survey information. It is designed to be used both as a software reference text and tutorial guide. The ESAP-95 software package currently contains three programs: ESAP-RSSD, ESAP-Calibrate, and ESAP-SaltMapper. The ESAP-RSSD program is designed to generate optimal soil sampling designs from bulk soil electrical conductivity survey information. The ESAP-Calibrate program is design to estimate both stochastic (regression model) and deterministic (soil theory based) calibration equations; i.e., the equations which are ultimately used to predict the spatial values of one or more soil variables from conductivity survey data. The final program, ESAP-SaltMapper, can be used to produce high quality 1D or 2D graphical output of conductivity survey data and/or predicted soil variables. This manual describes and documents the implementation and use of each of these three programs in detail.

George E. Brown Jr. Salinity Laboratory Research Report #146, 2000.

## **MODELING ARSENIC (III) ADSORPTION AND HETEROGENEOUS OXIDATION KINETICS IN SOILS**

**B.A. Manning and D.L. Suarez**

Arsenite [As(III)] is a soluble and toxic species of arsenic that can be introduced into soil by geothermal waters, mining activities, irrigation practices, and disposal of industrial wastes. We determined the rates of As(III) adsorption, and subsequent oxidation to arsenate [As(V)], in aerobic soil-water suspensions using four California soils. The rate of As(III) adsorption on the soils was closely dependent on soil properties that reflect the reactivity of mineral surfaces including citrate-dithionite (CD) extractable metals, soil texture, specific surface area, and pH. Heterogeneous oxidation of As(III) to As(V) was observed in all soils studied. The recovery of As(V) from As(III)-treated soils was dependent on levels of oxalate-extractable Mn and soil texture. After derivation of rate equations to describe the changes in soluble and recoverable As(III) and As(V) in soil suspensions, soil property measurements were used to normalize the empirically derived rate constants for three soils. The fourth soil, which had substantially different soil properties from the other three soils, was used to independently test the derived soil property-normalized model. The soil property-normalized consecutive reaction model gave a satisfactory description of the trends seen in the experimental data for all four soils. Understanding the effects of soil properties on the kinetics of chemical reactions of As(III) and As(V) in soils will be essential for development of quantitative models for predicting the mobility of As in the field.

Soil Sci. Soc. Am. J. 64(1):128-137, 2000.

## **USE OF EXAFS-DERIVED OXYANION SURFACE STRUCTURES IN A SURFACE COMPLEXATION MODEL**

**B.A. Manning, D.L. Suarez and S.E. Fendorf**

Oxanion surface structures derived from extended x-ray absorption fine structure spectroscopy (EXAFS) have been used to constrain the chemical description of the mineral-water interface in a surface complexation model. Arsenic(III) and (V) species were reacted with several synthetic minerals, well-characterized clays, and soil clay fractions followed by EXAFS analysis and wet chemical speciation using high performance liquid chromatography. This approach allowed simultaneous determination of solid-water partitioning data and solid phase analysis. Structural parameters developed in EXAFS data analysis software such as As-Fe and As-Al interatomic distances were then incorporated into the surface complexation model. Data from EXAFS suggested that a suite of adsorption sites (surface site heterogeneity) occurs on crystalline materials and thus extrapolation to soil will require simplifying assumptions.

Agronomy Abstract p. 214, 1999.

## **METHODS AND INTERPRETATION OF ELECTRICAL CONDUCTIVITY MEASUREMENTS**

**J.D. Rhoades, F. Chanduvi and S.M. Lesch**

The technology described in this report for measuring soil salinity has been extensively and successfully field-tested. It is concluded to be sound, reliable, accurate and applicable to a wide variety of useful applications. It is based on proven theory of soil electrical conductivity. The required equipment is commercially available. The advocated instrumental methodology is practical, cost effective and well developed for essentially all general applications. It is cheaper, faster and more informative than traditional methods of salinity measurement based on soil sampling and laboratory analyses. Software is available to facilitate its use for mapping and monitoring uses, as is equipment to mobilize and automate the measurements for use in detailed field-scale assessments. Its usefulness has been demonstrated: 1) for diagnosing soil salinity, 2) for inventorying soil salinity, 3) for monitoring soil salinity, 4) for evaluating the adequacy and appropriateness of irrigation and drainage systems and management practices, 5) for determining the areal sources of excessive leaching, drainage and salt-loading in crop lands, 6) for establishing the spatial soil information needed to develop prescription farming plans to manage fields with spatially-variable salinity conditions, and 7) for scheduling and controlling irrigations under saline conditions. It offers the potential to identify the inherent causes of salinization in fields, especially when integrated with GIS technology, and to identify mitigation needs, especially when integrated with field-scale deterministic, solute transport models. The salinity assessment approach advocated in this report offers a more suitable basis for evaluating, managing and controlling soil salinity than do the leaching requirement and salt balance concepts/measurements as traditionally applied. National programs need to be implemented to mitigate the substantial problems of secondary salinization that threatens the sustainability of irrigation in many places in the world. Holistic; meaningful salinity assessment approaches needed in this regard are illustrated in this report. The presented salinity assessment technology offers substantial practical potential to inventory, monitor, manage and control soil and water salinity, as will be needed to sustain irrigated agriculture and to meet the worlds food needs in the coming decades.

In: FAO Irrigation and Drainage Paper 57, Soil Salinity Assessment, Food & Agriculture Organization of the United Nations, Rome, 1999.

## **IMPACT OF AGRICULTURE ON CO<sub>2</sub> FLUXES AS AFFECTED BY CHANGES IN INORGANIC CARBON**

**D.L. Suarez**

Agricultural practices merit examination for their potential to alter global changes in C fluxes, due to their large impact on the land surface, as well as the large storage of C in soils (about 500 times the net yearly increase in atmospheric CO<sub>2</sub> as a result of fossil fuel burning). In this study we examine inorganic C reactions in agricultural soils, including mineral weathering, irrigation of surface and ground waters, liming of acid soils, and application of N fertilizers. Calculations of the impact of these processes for the U.S. and estimation of global effects indicates that although these processes result in net emissions, the effects are less than 1% of the calculated fossil fuel emissions. Potential for changing these C fluxes from inorganic C changes, is relatively low. Assuming to other climatic changes, doubling of the atmospheric CO<sub>2</sub> concentration will also have a minor impact on the net inorganic C fluxes from these agricultural processes.

In: R. Lal, J.M. Kimble, H. Eswaran and B.A. Stewart (eds.) *“Global Climate Change and Pedogenic Carbonates”*, Chapter 16, p. 257-272, CRC Press, Boca Raton, FL, 1999.



## **TRANSFORMATIONS OF VOLATILE METHYLATED SELENIUM IN SOIL**

**D.A. Martens and D.L. Suarez**

Microbial volatilization of selenium (Se) as dimethylselenide (DMSe) and dimethyldiselenide (DMDSe) from soil is an important part of the Se cycle in nature, but little is known about the stability and transformations of these gases during residence in the soil environment before dissipation to the atmosphere. Experiments monitored by gas chromatography and atomic absorption spectroscopy were conducted with various clay mineral standards, charcoal, commercial humic substances and soils to determine the sorption and transformations of DMSe and DMDSe injected into the headspace or passed through soil materials. Batch experiments conducted with 2 to 5 g materials placed into 40 mL Teflon centrifuge tubes equipped with Mininert<sup>TM</sup> gas sampling valves showed that DMSe was slowly sorbed by soil materials and the majority of the DMSe deficit in the headspace was recovered as  $\text{SeO}_3^-$  and  $\text{SeO}_4^{2-}$ . In contrast, DMDSe was rapidly partitioned from the gas phase and resulted in an increased recovery of less soluble elemental and selenide-Se forms. These results were confirmed during flow-through soil column studies with both little DMSe sorption and sorption of the majority of DMDSe addition. Additions of selenomethionine (SeMet) to soil to produce DMSe and DMDSe in sealed flasks resulted in an increased partitioning of Se into inorganic Se when compared with a flow-through system designed to limit the contact of Se gases with soil. These results suggest that soil Se volatilization as DMSe and DMDSe results in Se loss to the atmosphere as DMSe with concomitant soil Se immobilization due to the instability of DMDSe.

Soil Biology & Biochemistry 31:1355-1361, 1999.

## **SELENIUM IN WATER MANAGEMENT WETLANDS IN THE SEMI-ARID WEST**

**D.A. Martens and D.L. Suarez**

The discovery in 1983 of deformities, reproductive failures and high waterfowl mortality rates at Kesterson National Wildlife Refuge, western San Joaquin Valley, CA, due to selenium (Se) contaminated drainage water, raised concerns that these problems may be occurring in the >600 wetlands and National Wildlife Refuges being utilized to collect irrigation drainage waste water in 17 western states. The waterfowl problems were traced to ingestion of organic Se present as Se-amino acids. Plants assimilate soluble Se into Se-amino acids and release them upon decomposition. Aerobic plant residue decomposition studies showed that 50% of the assimilated Se was mineralized to soluble Se while the remaining organic Se persisted. This means that each growth cycle results in a steady decrease of soluble Se and an increase in organic Se levels. To test the effect of plant growth on Se accumulation, two types of evaporation ponds were evaluated, one with prolific plant growth and the second, relatively devoid of plant growth. Soil Se analysis showed that plant growth dramatically increased Se accumulation in the surface layers. Evaluation of additional Se-contaminated sites showed that Se accumulation followed an exponential function and accumulated rapidly above a 2% soil organic C content. Without plant growth, the Se remains mobile and diffuses to low concentrations in the underlying soil suggesting that plant residue cycling is an important factor in Se accumulation and toxicity.

Symposium: Wetlands and Horticulture: Problems and Solutions. 93rd ASHS Meeting, Lexington, KY, HortScience, 34:34-49, 1999.

## **EXTENT, CAUSE AND MANAGEMENT OF SALINITY IN THE U.S.A.**

**D.L. Suarez**

Increasing demands for high quality water by municipal and industrial users can no longer be met with development of new water supplies in the western U.S. If irrigated agriculture in the western U.S. is to maintain its important role in food production, agriculture will have to utilize lower quality water for irrigation, including reuse of drainage water, use of treated municipal waste waters and development of brackish waters presently considered undesirable for irrigation. The causes of salinity problems in the U.S. are varied, ranging from the presence of saline geologic formations, such as the shales of Colorado and Utah, presence of saline ground water in the upper Great Plains (Dakotas, and north western Colorado) and irrigated areas with either insufficient drainage or non-optimum water management. Salinity problems have been aggravated by excessive rather than insufficient irrigation or infiltration. Increased use of low quality water and implementation of drainage water reuse will require not only improved water management but also application of periodic salinity monitoring and prediction of the impact of management changes on salinity, crop production and soil physical properties. Changes in management practices, such as cyclic reuse of drainage water or supplemental irrigation with low quality waters can now be evaluated using process-based computer models that consider the dynamics of water flow including irrigation amounts and timing, crop water requirements, and sensitivity to water and salt stress, and solution chemistry including the effects of chemistry on soil physical properties. New management practices are needed for minimizing the adverse impact of drainage return flows including toxic anions.

In: Water Reports, Soil Management for Sustainable Use of Salt Affected Soils, Food & Agriculture Organization of the United Nations, (in press) 2000.

## **SELENATE AND SELENITE SORPTION ON IRON OXIDES: AN INFRARED AND ELECTROPHORETIC STUDY**

**C. Su and D.L. Suarez**

We studied selenate and selenite sorption by amorphous Fe oxide [am-Fe(OH)<sub>3</sub>] and goethite ( $\alpha$ -FeOOH) as a function of time (25 min-96 h), pH (3-12), ionic strength (0.01-1.0 *M* NaCl), and total Se concentration (0.0001-1.0 *M*). We examined sorbed selenate and selenite by in situ attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy, diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy, and electrophoresis to deduce sorption mechanisms. Sorption of both selenate and selenite reached equilibrium in <25 min and the sorption isotherm was not reversible. Increasing ionic strength decreased selenate sorption but did not affect selenite sorption. The presence of either selenate or selenite lowered the electrophoretic mobility (EM) and decreased the point of zero charge (PZC) of both sorbents, suggesting inner-sphere complexation for both selenate and selenite species. Both in situ ATR-FTIR and DRIFT difference spectra showed bidentate complexes of selenate with am-Fe(OH)<sub>3</sub>. The structure of selenite complexes in am-Fe(OH)<sub>3</sub>- solution interface was uncertain due to insensitivity of the in situ ATR-FTIR technique. The DRIFT spectra of selenite on am-Fe(OH)<sub>3</sub> showed  $\nu_3$  splitting as evidence of complexation. The DRIFT spectra of selenite on goethite showed bridging bidentate complex of selenite. We conclude that the influence of ionic strength on Se sorption cannot be used as a criterion for distinguishing outer- vs. inner-sphere complex formation.

Soil Sci. Soc. Am. J. 64(1):101-111, 2000.

## **THE FUTURE OF SOIL MANAGEMENT FOR SALINITY CONTROL**

**D.L. Suarez**

Increasing competition for scarce water resources will result in the use of lower quality water for irrigation. There is also increased environmental concern about off-site impacts of drainage waters. These factors result in increased salinity hazard thus the need to improve management. Evaluation of salinity status is possible with rapid EM measurements in combination with GPS information and GIS for rapid signal processing and display of results. Improved evaluation of management options will be possible with development of user friendly computer simulation models that are compatible with the type and data structure of the sensing equipment, and that incorporate the detailed processes of water distribution, infiltration and transport, chemical reactions and plant water uptake and growth. Such integrated tools will allow us to utilize precision farming concepts for salinity management, taking into account the spatial variation in soil properties, salinity and chemistry and improving water distribution while minimizing drainage return flows.

Agronomy Abstract p. 285, 1999.

## **IMPACT OF IRRIGATED AGRICULTURE ON SOIL CARBON STORAGE IN COLORADO RIVER BASIN**

**D.L. Suarez**

Agricultural practices may result in both addition or removal of inorganic and organic carbon from soils. Interest in characterizing changes in inorganic carbon as a result of irrigation stem from both the large quantities of inorganic carbon in soils as well as model calculations suggesting large amounts of carbonate precipitation. Soil cores were taken from Grand Valley, Palo Verde Valley and Imperial Valley, all irrigated with Colorado River water for up to 110 y. Matched cores (irrigated and never irrigated) were taken from adjacent locations. Samples were analyzed with depth for soil texture, inorganic carbon, organic carbon and carbon isotopic composition. Analysis of these cores indicated no significant differences in the inorganic carbon and minor differences in the organic carbon content of the irrigated and adjacent non-irrigated soils. Consistent with these results, the stable C isotopic analyses indicated that almost all the carbonate was of marine origin. The slightly lighter  $^{12}\text{C}/^{13}\text{C}$  isotopic ratio in some of the irrigated sites is consistent with minor amounts of re-precipitated calcite as a result of wetting and drying cycles associated with irrigation practices. These data are not consistent with steady state models of carbonate precipitation based on estimated leaching fractions, that predict large increases in inorganic carbon storage as a result of irrigation in the lower Colorado River basin. Experimental data were also compared to results from simulations using the UNSATCHEM model. Consideration of the dynamics of  $\text{CO}_2$  root zone transport and concentrations, calcite precipitation kinetics and additions of  $\text{NH}_4$  fertilizers suggest that limited precipitation may occur lower in the soil profile. Mass balance calculations based on alkalinity in irrigation and drainage water are consistent with inorganic carbon precipitation. Additional measurements in these and other basins, including deeper subsurface samples are needed to quantify the impact of irrigation on carbon storage in semi-arid and arid lands.

Advances in Terrestrial Ecosystem Carbon Inventory, Measurements, and Monitoring, Raleigh, NC, Abstr., 2000.

## **MODELING IRRIGATION WITH LOW QUALITY WATERS AND SODIC SOIL RECLAMATION**

**D.L. Suarez**

Existing water quality criteria for irrigation consider salinity and the sodium adsorption ratio. These parameters reflect the adverse effect of Na (and low salinity) on soil hydraulic properties, but do not consider the infiltration rates required for specific crop and climatic conditions nor the achievable infiltration rates under actual field conditions. Similarly, chemical transport models that consider plant water uptake have been utilized for predicting the long term effects of irrigation on chemical parameters, but the effects on hydraulic characteristics have not been incorporated into these models. The UNSATCHEM model has unique capabilities including CO<sub>2</sub> production and transport routines for dynamic prediction of pH as well as consideration of the effects of chemical properties, including pH, on soil hydraulic characteristics and infiltration. Soil and management-specific information is required to enable simulation of the site-specific conditions. Examples of the use of the model are provided from field and laboratory studies of sodic soils from Coachella, CA. Simulations of irrigation on sodic soils illustrates the importance of soil texture and related hydraulic and chemical properties on ease of reclamation. Reclamation schemes can be evaluated in terms of amounts of amendments, water and time required for restoration of adequate infiltration. Similarly irrigation with low quality water may not result in immediate adverse effects on infiltration and salinity but long term effects may be very adverse. Since long term effects are not easily measured experimentally, there is need for conceptual understanding of the processes and subsequent model simulation of the time-dependent processes.

Sodicity Issues in Agricultural Industries-Current Research and Future Directions, in Tatura, Victoria, Australia, Abstr., 2000.

## **UNSATCHEM3.0 WATER AND MULTICOMPONENT CHEMICAL TRANSPORT WITH WINDOWS USER INTERFACE**

**D. L. Suarez, P.J. Vaughan and S.M. Lesch**

The UNSATCHEM model has been updated with inclusion of additional chemical capability, conversion to 32 bit double precision code and a Windows based interface. The interface consists of a pre and post processor with graphing capability. In addition to the previous capabilities to predict CO<sub>2</sub> production and transport, variably saturated water flow, heat flow major ion cation exchange and precipitation-dissolution of calcite, gypsum and Mg carbonates, the model now includes consideration of calcite precipitation kinetics including the inhibiting effect of DOC on precipitation, capability to consider multisite cation adsorption, enabling prediction of cation selectivity based on organic matter and clay mineral content, B chemistry and adsorption using the constant capacitance model, silicate mineral weathering, including feldspars, micas and hornblende, and calculation of  $E_t$  using crop coefficients and the Penman Monteith equation. The model is freely available and includes a user manual.

Agronomy Abstract p. 41, 2000.



## **PREDICTION OF B TRANSPORT IN SOIL COLUMNS**

**D.L. Suarez**

Reuse of agricultural and municipal waste waters are often limited by the elevated concentrations of B. Use of these water requires ability to predict the B concentration in solution with time, as well as development of effective reclamation practices. Existing B transport models require detailed soil-specific B adsorption- desorption characterization or empirical fitting of  $K_d$  parameters. This study compares the predictive capability of the UNSATCHEM model utilizing surface area to estimate the surface site density (moles/g) and generalized constant capacitance parameters. Three arid land soils were packed into soil columns, reacted with 0.08 mmol/L B solutions at pH 6 and pH 9, and subsequently leached with pH 6 and 9, B- free water. At elevated pH B adsorption increased and desorption was decreased relative to pH 6. The model was able to adequately predict B concentrations during both adsorption and desorption without the need to characterize the sorption characteristics of each soil. The greatest uncertainty in predicting B concentrations was associated with fluctuations in soil pH.

Agronomy Abstract p. 230, 2000.

## **ROLE OF GROUNDWATER FLOW IN TILE DRAIN DISCHARGE**

**P.J. Vaughan, D.L. Suarez, J. Šimůnek, D.L. Corwin and J.D. Rhoades**

Tile systems drain water applied to agricultural fields as irrigation and precipitation but also may intercept regional groundwater flow. Identification and characterization of the potential sources of tile water is essential for informed management of salinity and contaminants. Factors influencing tile discharge including depth of water applied, evapotranspiration, water storage, drain blockage, and interception of regional groundwater flow were evaluated to determine which may be related to a fivefold variation in cumulative tile discharge among six sumps located 100 km west of Fresno, CA. Cumulative depths drained were calculated for 5 yr of weekly irrigation, precipitation, and discharge data. Evapotranspiration and water storage were estimated using the UnsatchemGeo variably-saturated water flow model. Well water levels measured on 19 dates were spatially-averaged providing spatial variation of depth-to-water among the drained areas. Variability in depth of water drained (0.18-0.95 m) was large and was not correlated with either water applied (3.26-4.58 m,  $r^2=0.03$ ) or with computed water flux from the bottom of the soil column (0.05-0.31 m,  $r^2=0.00$ ). Groundwater interception by tile drains was a factor because depth-to-water was negatively correlated with discharge ( $r^2=0.42$ ) and drawdown of groundwater levels by drains was relatively larger for those drained areas encountered first during regional groundwater flow. For all six sumps, drained water is likely derived from locally applied water and interception of regional groundwater flow implying that standard two-dimensional models of flow to drains, representing only water applied locally, would not be applicable to modeling of drain flows or drain-water solute concentrations.

J. Environ. Qual. 28(2):403-410, 1999.

## **ABOVE-CANOPY CO<sub>2</sub> FLUX FOR WHEAT IN CENTRAL OKLAHOMA: A COMPARISON OF MODEL RESULTS WITH MEASURED DATA**

**P.J. Vaughan and D.L. Suarez**

At AmeriFlux sites CO<sub>2</sub> flux is measured continuously to provide information about the processes and extent of carbon sequestration in the soil in different ecosystems. A data set consisting of meteorological measurements made every half-hour at a height of 4.5 m at the AmeriFlux Wheat Site in Oklahoma was processed to remove all gaps in the data to prepare it for modeling. The 1-D Unsatchem model was linked to the GAS-FLUX layered canopy gas exchange model to make the USGF combined model. Photosynthesis model parameters for canopy gas exchange were published values of single-leaf gas exchange in wheat. Parameter values for the subsurface CO<sub>2</sub> production model were the same as those used in earlier modeling of soil surface CO<sub>2</sub> flux in wheat by Unsatchem. When the scaling constants for photosynthesis in light-saturated and light-limited conditions were adjusted to optimal value, predictions of CO<sub>2</sub> flux matched measured flux. The Wheat site was located within the ARM-CART SGP97 area, the wheat-growing areas were classified by the SGP97 project. A subarea surrounding the Wheat site was selected for estimation of daily net carbon balance occurring in wheat. The calculation indicated net CO<sub>2</sub> loss in this area during 1996-97 but uncertainty suggests that making CO<sub>2</sub> surface flux measurements could provide additional constraints on the subsurface CO<sub>2</sub> production.

4th International Conference on Integrating GIS & Environmental Modeling (GIS/EM4), Available at the following web site: <http://www.Colorado.edu/research/cires/banff/upload/75>, 2000.

## **ATMOSPHERIC CO<sub>2</sub> FLUX PREDICTION BY USGF MODEL FOR AMERIFLUX WHEAT SITE**

**P.J. Vaughan, R.J. Ryel, D.L. Suarez and C.W. Rice**

The Unsatchem model of water flow, CO<sub>2</sub> transport and multicomponent solute transport in the vadose zone was linked to the GAS-FLUX canopy photosynthesis and transpiration model to generate the USGF model of combined plant and soil processes. Linkage includes feedback of the mean water pressure head within the root zone to the plant model through reduction of the maximum stomatal conductance by a water stress factor. Transpiration calculated in the GAS-FLUX component determines root water uptake. Data required by USGF include solar radiation, precipitation, weather data, photosynthesis model parameters and plant structure such as LAI and leaf angles for different levels in the canopy. Predictions include water and CO<sub>2</sub> flux above the canopy. Data collected at the Ameriflux Wheat site (OK) during 9/96-8/97 at 30-minute intervals are sufficiently detailed for comparison of model results with measured flux data.

Agronomy Abstract p. 15, 1999.

## **NET ECOSYSTEM EXCHANGE CALCULATED FOR THE AMERIFLUX WHEAT SITE, OKLAHOMA**

**P.J. Vaughan and D.L. Suarez**

Net ecosystem exchange measured at the AmeriFlux Wheat Site in Oklahoma by the eddy covariance technique was compared to model results obtained from the USGF combined model of canopy gas exchange and subsurface CO<sub>2</sub> production and transport. The simulations were run for a 352-day period in 1996-97 that overlaps the winter wheat growing season. The advantage of using CO<sub>2</sub> flux to calculate carbon storage instead of simply measuring the changes in soil carbon concentration is that the length of the simulation required for calculating a meaningful change in carbon storage is much shorter. Preliminary results suggest that there was a small loss of carbon from the subsurface during the 352-day period. These simulations suggest that measurement of CO<sub>2</sub> surface flux could provide a useful complement to above-canopy CO<sub>2</sub> flux enabling more accurate parameterization of the subsurface CO<sub>2</sub> production and transport model. Application of the model to various ecosystems is possible and desirable because the model could be used for making spatial predictions of carbon sequestration that, being based on calculation of carbon flux, would provide a sensitive estimation as compared to a carbon-pool type of model.

Advances in Terrestrial Ecosystem Carbon Inventory, Measurements, and Monitoring. Raleigh, NC, Abstr., 2000.

## **PARAMETERIZATION OF LINKED CANOPY GAS EXCHANGE AND SOIL PROCESS MODEL**

**P.J. Vaughan**

Atmospheric CO<sub>2</sub> flux, measured at the AmeriFlux Wheat Site in Oklahoma, was compared to predictions of above-canopy flux by a linked model of canopy gas exchange and subsurface CO<sub>2</sub> production and transport. A standard error of the estimate (sigma) was computed for year-long simulations utilizing different sets of model parameter values. Calculation of net photosynthesis in the canopy gas exchange model required calculation of V<sub>cmax</sub>, the maximum carboxylation rate, and P<sub>m1</sub>, the CO<sub>2</sub>- and light-saturated rate of photosynthesis. By varying the scaling factors (F<sub>vc</sub> and C) in the Johnson-Eyring expressions for these two rates, a surface representing sigma on a plot of F<sub>vc</sub> vs. C was found to have two orthogonal minimum branches. This shape occurred because the modeled light-response curve had nearly the same form for different (F<sub>vc</sub>,C) pairs along the minimum in sigma. Other parameters that were studied include the activation energy and scaling factor for dark respiration, quantum efficiency, and leaf angle.

Agronomy Abstract p. 28, 2000.